

Pentyl 2-hydroxypropanoate
6382-06-5 | DTXSID70858752

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.62

Global applicability domain: Inside

Local applicability domain index: 4.79e-01

Confidence level: 7.19e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Isopropyl-6-methyl-4-pyrimidone</div> <div>Measured: 1.82</div> <div>Predicted: 2.23</div>	<div>Image not found</div> <div>Acetamide, N-methyl-N-phenyl-</div> <div>Measured: 1.51</div> <div>Predicted: 2.53</div>	<div>Image not found</div> <div>Bromacil</div> <div>Measured: 3.24</div> <div>Predicted: 2.87</div>
<div>Image not found</div> <div>1,8-Naphthalenediamine</div> <div>Measured: 6.31</div> <div>Predicted: 3.19</div>	<div>Image not found</div> <div>1,3-Benzenedimethanamine</div> <div>Measured: 2.69</div> <div>Predicted: 4.58</div>	